Supplementary Material (ESI) for New Journal of Chemistry

SUPPLEMENTARY INFORMATION

Table 1. ^{1}H NMR chemical shifts of CH protons of catechins **1** – **4** (δ, ppm) and complexation induced shifts (CIS) when in complex with β-CD in D_2O at 298 K.

		H2	H3	H4α	H4β	H6	H8	H2'	H5'	H6'	H9',13'
C (**1**)	δ	4.151	4.7	2.467	2.792	6.021	5.941	6.861	6.842	6.784	
	CIS	−0.068	a	0.106	a	−0.016	−0.094	−0.139	−0.172	−0.152	
EC (**2**)	δ	4.235	4.897	2.685	2.839	6.027	6.005	6.955	6.855	6.855	
	CIS	−0.029	−0.059	−0.037	0.047	−0.052	−0.111	−0.033	0.026	−0.034	
EGC	δ	4.218	4.831	2.678	2.827	6.023	6.005	6.547		6.547	
(**3**)	CIS	−0.012	−0.102	0.039	0.049	−0.041	−0.068	0.008		0.008	
EGCG	δ	5.030	5.516	2.841	2.972	6.074	6.042	6.496		6.496	6.899
(**4**)	CIS	−0.211	−0.214	0.019	0.246	−0.138	−0.136	0.223		0.223	0.109

a. Not visible in the NMR spectrum.

Table 2. ^{1}H NMR chemical shifts of CH protons of β-CD alone (δ, ppm) and complexation induced shifts (CIS) when in complex with catechins in D_2O at 298 K.

β-CD		H-1	H-2	H-3	H-4	H-5	H-6
	δ	4.978	3.557	3.874	3.492	3.786	3.786
C (**1**)	δ'	4.941	3.529	3.806	3.481	3.593	3.677
	CIS	−0.037	−0.028	−0.068	−0.011	−0.193	−0.109
EC (**2**)	δ'	4.948	3.529	3.808	3.493	3.692	3.717
	CIS	−0.03	−0.028	−0.066	0.001	−0.094	−0.069
EGC (**3**)	δ'	4.954	3.535	3.824	3.497	3.703	3.712
	CIS	−0.024	−0.022	−0.05	0.005	−0.083	−0.074
EGCG (**4**)	δ'	4.943	3.533	3.769	3.485	3.687	3.710
	CIS	−0.035	−0.024	−0.105	−0.007	−0.099	−0.076

Table 3. ROE between C (**1)** (5 mM) and β-CD (5 mM) in D_2O at 298 K.

CD	H-3	H-5	H-4
H2	W [c]		
H3		M	
H4	M		
H6	S		
H8	S		
H2’	W		W
H5’	S [a]	M	S
H6’	S		M [b]

ROE between EC (**2)** (5 mM) and β-CD (5 mM) in D_2O at 298K.

CD	H-2	H-3	H-5	H-6
H4	M	M	M	M
H6		W	S	
H8	W	W	S	
H2’	W	S	M	W
H5’	W	M	M	W
H6’	W	M	M	W

ROE between EGC (**3)** (5 mM) and β-CD (5 mM) in D_2O at 298K.

CD	H-2	H-3	H-5	H-6
H2		M		
H3		S		
H4		M	W	
H6		M		
H8	W	S	M	M
H2’,6’	W	S	M	W

[a, b, c] S, strong; M, medium; and W, weak.

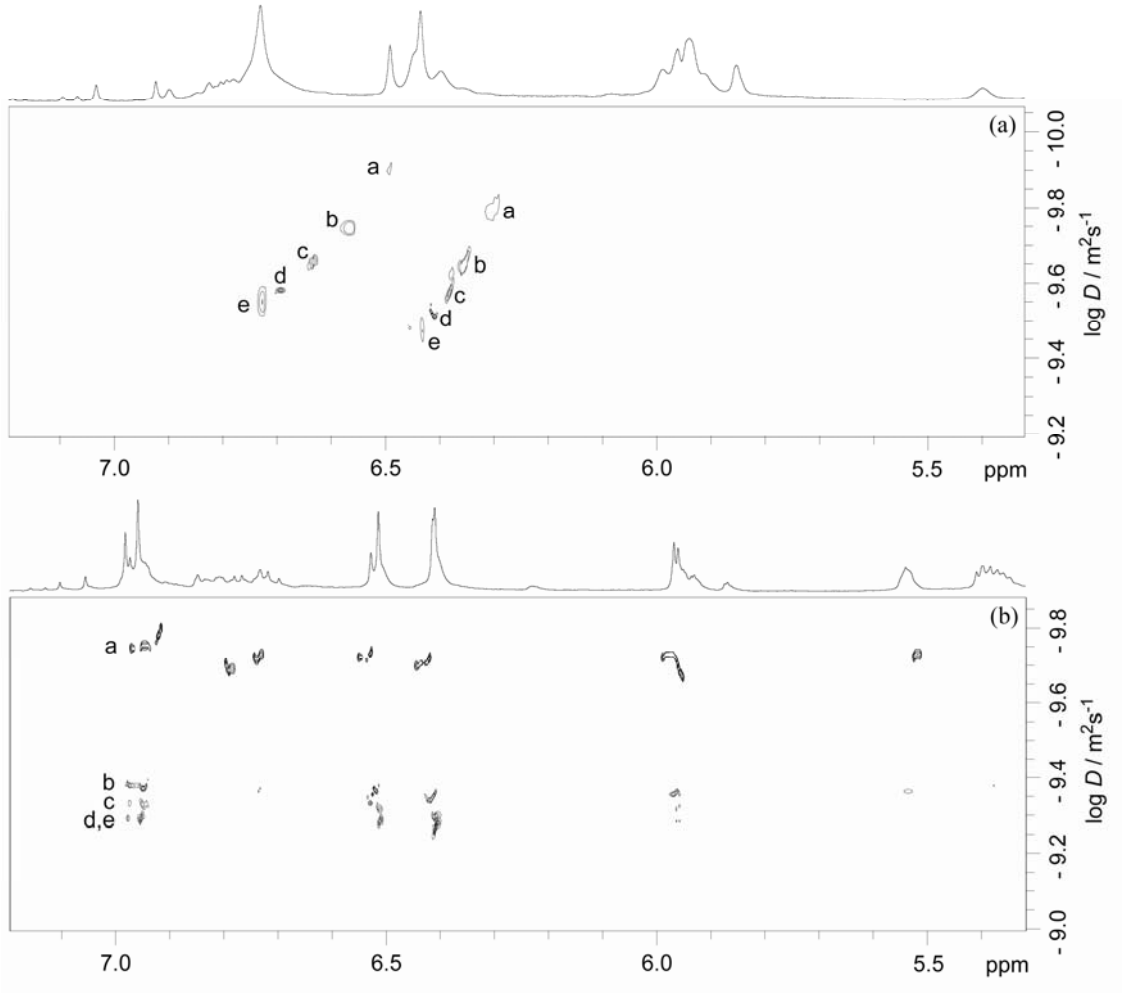

Figure 1. DOSY spectra of GTE showing the influence of viscosity on the diffusion coefficient. (A) Water extraction: a) concentrated sample, b) half concentration of sample a), c) 100 mg/mL, d) 50 mg/mL, e) 12 mg/mL (B) Methanol extraction: a) concentrated sample, b) 50 mg/mL, c) 25 mg/mL, d) 12 mg/mL, e) 6 mg/mL. The one-dimensional ^{1}H NMR spectra shown on the top of the DOSY spectra are those of sample e.